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# Electric Dipole Polarizabilities of Hydrogen and Helium Isotopes

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The electric dipole polarizabilities of <sup>3</sup>H, <sup>3</sup>He, and <sup>4</sup>He are calculated directly using the Schrödinger equation with the latest generation of two- and three-nucleon interactions. These polarizabilities are necessary in order to obtain accurate nuclear-polarization corrections for transitions involving S-waves in one- and two-electron atoms. Our results are compared to previous results, and it is shown that direct calculations of the electric polarizability of <sup>4</sup>He using modern nuclear potentials are smaller than published values calculated using experimental photoabsorption data. The status of this topic is assessed in the context of precise measurements of transitions in one- and two-electron atoms.

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### I. INTRODUCTION

Calculations of Quantum Electrodynamic (QED) corrections have reached a level of precision in hydrogenic atoms and ions where (much smaller) nuclear corrections are necessary in order to interpret some high-precision measurements of transition frequencies[1–3]. In many cases the experimental errors and estimated sizes of uncalculated QED corrections are much smaller than the nuclear corrections, and one can thus use those measurements (corrected for QED effects) as an experimental determination of various nuclear quantities[4, 5]. We briefly review several such determinations.

For S-wave hyperfine transitions in one-electron atoms and ions[5-7], experimental precision is much greater than that of all theoretical calculations, while uncalculated theoretical contributions to transition frequencies (including QED corrections) are significantly smaller than nuclear effects. The leading-order (i.e., largest) nuclear contribution to these hyperfine transitions (called a Low moment[8]) is determined by a correlation between the nuclear charge and current operators [6, 7]. Low moments may be further decomposed into Zemach moments[9] (viz., utilizing only ground-state expectation values of the charge and current operators) and polarization contributions (viz., including only virtual excited states between the two operators), both of which play significant roles. For the important proton (i.e., <sup>1</sup>H) case the polarization effects are significantly smaller than the static (Zemach) corrections because the proton is much more difficult to excite than any nucleus[10–12]. Although exceptionally interesting, hyperfine transitions are not the focus of this note.

The frequencies of transitions between S-states in hydrogenic atoms and ions can be separated into a reference value (essentially the Dirac transition frequency

modified by reduced-mass effects) plus the much smaller Lamb shift. The Lamb shift contribution is dominated by QED corrections, but nuclear effects play a significant role in the best measured transitions. These nuclear corrections can be decomposed into nuclear finite-size corrections (i.e., determined by nuclear ground-state charge distributions) plus nuclear polarization corrections (viz., involving virtual excited states of the nucleus). The latter are typically dominated by the electric polarizability, which reflects the distortion of the nuclear charge distribution as it is attracted by (and follows) the orbiting electron.

The most accurate measurement of such a frequency was performed in Ref.[13] for the 1S-2S transition in hydrogen, with a relative error of slightly more than 1.4 parts in  $10^{14}$  and with an absolute error of 34 Hz. That error is slightly smaller than the estimated polarization correction of 60(11) Hz from Ref. [14], and is much smaller than the size correction of about 1000 kHz. The mismatch in the sizes of these corrections again reflects the fact that the proton is difficult to excite (compared to a nucleus), but its size is not significantly smaller than that of light nuclei. If one turns the problem around and extracts the proton-size correction from the experimental transition frequency, one obtains a value for the proton r.m.s. charge radius of  $\langle r^2 \rangle_{ch}^{1/2} = 0.877(7)$  fm[1], which agrees with a recent direct determination of that quantity from elastic electron-scattering data:  $\langle r^2 \rangle_{ch}^{1/2} =$ 0.897(18) fm [15, 16]. Both the polarization-correction and experimental errors are much smaller than the Rydberg constant error, which dominates the uncertainty in the hydrogen atom analysis.

A similar analysis[1] of transitions from the 2S state in deuterium to a variety of S and D states leads to a value of the deuteron charge radius of  $\langle r^2 \rangle_{ch}^{1/2} = 2.1402(28)$  fm, which is consistent with the electron scattering value[17, 18] of  $\langle r^2 \rangle_{ch}^{1/2} = 2.130(10)$  fm. Note that this is the full charge radius (in contrast to the quantity discussed next), and that the atomic value has an uncertainty nearly 4 times smaller than the value obtained

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directly from electron scattering.

The determination of the difference in transition frequencies between hydrogen and deuterium can be used to test our understanding of small contributions to the charge radius of the deuteron[4]. Because the finite size of the proton contributes linearly to the deuteron meansquare radius (which determines the dominant nuclearsize correction in an atom), it largely cancels out in the frequency difference. Higher-order proton-size corrections and neutron-size corrections are relatively small and tractable. The transition-frequency difference (dominated by calculable reduced-mass effects) was reported in ref.[19] for 1S-2S transitions with a relative accuracy of 2.2 parts in  $10^{10}$ , and with an absolute error of 0.15 kHz. The nuclear electric polarizability of deuterium contributes 19.26(6) kHz [20], which is more than two orders of magnitude greater than the experimental error, while the deuteron-size correction is greater than 5000 kHz. The weak binding of the deuteron makes possible the calculation of the bulk of the polarization and nuclearsize corrections in terms of a few well-measured parameters. The tiny remaining size correction includes statistically significant contributions to the nuclear charge radius arising from meson-exchange currents and relativistic corrections [4, 21], which are unobtainable from other types of experiments such as electron scattering. Obtaining this sensitivity to fine details of nuclear dynamics crucially depends on accurate estimates of the deuteron electric polarizability.

Measurements of S-wave transition frequencies in <sup>3</sup>H, <sup>3</sup>He, and <sup>4</sup>He atoms are not yet as accurate as those described above, nor are the necessary theoretical calculations for He atoms. Hopefully both can be improved [22] to the point where nuclear physics information can be extracted, particularly information about the r.m.s. charge radii. As reviewed and updated in Ref. [23], on the other hand, isotopic differences in transition frequencies for helium and singly ionized lithium isotopes now have the required experimental and theoretical sensitivity. The latter sensitivity is greatly enhanced by the cancellation of nuclear-mass-independent relativistic and QED corrections in isotopic differences. In complete analogy to the hydrogen-deuterium case, calculable reduced-mass effects dominate the frequency difference, leaving nuclear contributions as the residue after relativistic and QED contributions are subtracted. There has been considerable recent interest in the isotope shift of <sup>3</sup>He[24, 25], <sup>6</sup>He[26–28], and <sup>8</sup>He[28] transitions relative to those of <sup>4</sup>He. In each case values of the r.m.s. charge radius of those nuclei has been extracted relative to the charge radius of <sup>4</sup>He[29, 30]. The nuclear polarizability correction to the <sup>3</sup>He - <sup>4</sup>He isotope-shift frequency (the best measured of the He isotope shifts) is about 2/3 of the 3 kHz experimental uncertainty[23–25], while presently only a marginal influence [23] on the others, but future improvements should require reliable values of the electric polarizability (as was the case for the deuteron), and that is the purpose of this note.

#### II. CALCULATIONS

The electric polarizability of a nucleus (or atom) is defined by

$$\alpha_{\rm E} = 2\alpha \sum_{N \neq 0} \frac{|\langle N|D_z|0\rangle|^2}{E_N - E_0}, \qquad (1)$$

where  $E_0$  is the energy of the ground-state  $|0\rangle$ ,  $E_N$  is the energy of the N<u>th</u> excited state,  $|N\rangle$  (all of which are in the continuum for few-nucleon systems), and  $D_z$  is the component of the (non-relativistic, in our case) electric-dipole operator in the  $\hat{z}$  direction, which generates the transition between those states. The definition (1) can be rearranged into the form of a sum rule

$$\alpha_{\rm E} = \frac{1}{2\pi^2} \int_{\omega_{\rm th}}^{\infty} d\omega \frac{\sigma_{\gamma}^{\rm ud}(\omega)}{\omega^2} \equiv \frac{\sigma_{-2}}{2\pi^2} \,,$$
 (2)

where  $\sigma_{\gamma}^{\rm ud}(\omega)$  is the nuclear cross section for photoabsorption of unretarded-dipole (long-wavelength) photons with energy  $\omega$ , and  $\omega_{\rm th}$  is the threshold energy for photoabsorption. The inverse-energy weightings in Eqns. (1) and (2) lead to significant sensitivity of  $\alpha_{\rm E}$  to the threshold energy,  $\omega_{\rm th}$ , which depends on nuclear binding energies.

In order to obtain the nuclear energy spectra and the wave functions involved in the calculation of the electric polarizability (see Eqn. (1)), we use the no-core shell model (NCSM) in relative coordinates [31] to solve the Schrödinger equation. The NCSM is a flexible approach to solving the few- and many-nucleon problems, and it has been extensively used in studies of s- and pshell nuclei [32–36]. In the NCSM the nuclear wave functions are obtained by the diagonalization of an effective Hamiltonian in a finite basis constructed from harmonic oscillator (HO) wave functions. The truncation of the model space is taken into account via an effective interaction derived by means of a unitary transformation. Either local or non-local high-precision nucleon-nucleon (NN) and three-nucleon (NNN) interactions can be used in the Schrödinger equation. The effective interaction is constructed in a cluster approximation, which neglects many-body contributions. Errors associated with the cluster approximation are removed by observing the convergence of observables as a function of the number of basis states included in the calculation. The truncation of the model space is determined and labeled by the number of excitations,  $N_{max}$ , above the non-interacting state. Our convergence tests will plot calculated quantities vs.  $N_{max}$ , and those quantities should approach asymptotic values as  $N_{max}$  becomes infinite.

In this paper we compute the <sup>3</sup>H, <sup>3</sup>He and <sup>4</sup>He electric dipole polarizabilities starting from a nuclear Hamiltonian derived within the framework of (QCD-based) Chiral Perturbation Theory (including the Coulomb interaction between the protons). The nucleon-nucleon interactions were derived at next-to-next-to-next-to-leading order (or N<sup>3</sup>LO) [37], while the three-nucleon interactions were derived at next-to-next-to-leading order (or

 $\rm N^2LO)$  [38, 39]. The accuracy of these nuclear interactions for s- and p-shell nuclei was investigated extensively in the same NCSM framework in Ref. [34]. It was shown in Ref. [35] that the experimental binding energies of  $^3\rm H$  and  $^3\rm He$  were reproduced with high accuracy (viz., within 8 keV, or about one part per thousand), while Ref. [36] showed that the same nuclear potential produced a binding energy for  $^4\rm He$  that was too large by about 300 keV (approximately 1%). These modern nuclear forces therefore provide an accurate description of the structure of the nuclides considered here ( $^3\rm H$ ,  $^3\rm He$ , and  $^4\rm He$ ) as well as the total photoabsorption cross section of  $^4\rm He$  (discussed below).

For each nucleus we first solve the few-nucleon Schrödinger equation in order to obtain the ground-state wave function, which can be accurately described in a large HO basis. We next rearrange Eqn. 1 according to Podolsky's technique[40], which allows the ground state to be used as the driving term for the Lanczos-moment method [41, 42], which is our method of choice for solving the Schrödinger equation. This trick allows us to work only with bound-state quantities and to bypass the much more difficult approach of computing a response in the continuum. A detailed description of this method in a NCSM framework was given in Ref. [43].

Finally, we note that the same technique used to obtain the effective nuclear interaction should in principle be applied to the transition operator. Nevertheless, investigations of effective operators in the NCSM have shown that long-range operators (such as our dipole operator) require only very weak renormalization [44, 45] and for that reason we can work with the unrenormalized dipole operator.

# III. RESULTS AND COMPARISON WITH OTHER WORK

In Figs. 1–3, we show the running of the electric polarizability with the truncation parameter for the model space,  $N_{max}$ . Different HO parameters result in different convergence patterns for the electric polarizability and this fact is especially visible for small  $N_{\rm max}$  values. As shown in Figs. 1–3, results using smaller HO frequencies  $\omega$  converge faster. Thus, because smaller values for  $\Omega$ are equivalent with larger associated length parameters,  $b=1/\sqrt{m_N\Omega}$ , long range operators, such as the dipole transition operator, are better described in smaller model spaces. Moreover, better sampling of the low-lying excited states (the most important in the calculation of the electric polarizability) is obtained for small values of  $\Omega$ . While not shown, other operators converge faster at small HO frequencies. In particular for binding energies, the fastest convergence is achieved for a HO length parameter b of the order of the size of the nucleus considered. However, for large  $N_{max}$ , the results obtained with different frequencies of the HO basis approach a single asymptotic value, independent on the observable considered.

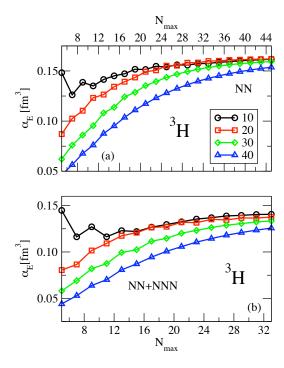


FIG. 1: [Color online] The dependence of (the electric polarizability)  $\alpha_E$  of <sup>3</sup>H (in units of fm<sup>3</sup>) on the model-space truncation parameter,  $N_{max}$ . The results have been obtained using (a) NN interactions only, and (b) NN+NNN interactions. Each curve is obtained using a different frequency parameter for the basis states, shown in the legend in MeV. For sufficiently large  $N_{max}$  each result should be independent of that frequency.

We present in the the upper panels of Figs. 1–3 results obtained neglecting three-body interactions, while results that include three-body forces are shown in the lower panels. Note, however, that because the binding energy is not correctly described in the absence of three-nucleon interactions, the values obtained with only NN interactions are about 10–25% larger than the results obtained when NNN interactions are included. This is largely the effect of having an incorrect value for  $\omega_{\rm th}$ .

Our calculations of the electric polarizabilities of threeand four-nucleon isotopes of hydrogen and helium are summarized in Table I, together with those of others using different two-nucleon and three-nucleon forces. We have restricted our own entries to those that incorporate three-nucleon forces and hence have accurate binding energies, especially for the three-nucleon systems and slightly less so for <sup>4</sup>He. The three-body parameters can be determined from different three-body data, and, while in the three-body system there is basically no change in the results, the binding energy of <sup>4</sup>He is slightly better described in one case. Consequently, the electric polarizability changes and this is why we present two values for the  $\alpha$  particles; see below for more details. In the case of <sup>4</sup>He, the two different values for the electric polarizability are obtained with two different strengths of the three-body forces. For completeness in the table we have

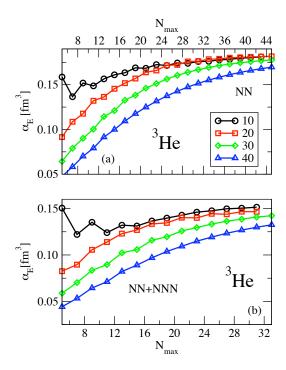


FIG. 2: [Color online] Same as in Fig. 1, but for <sup>3</sup>He.

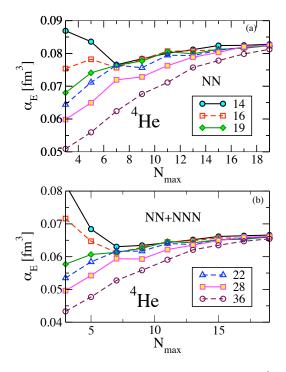


FIG. 3: [Color online] Same as in Fig. 1, but for <sup>4</sup>He.

also included the deuterium and  $^6\mathrm{He}$  cases, which were not treated in this work.

Only one other calculation of  $\alpha_{\rm E}$  for <sup>3</sup>H exists[46], and our result is in agreement with that calculation.

Calculations for the electric polarizability of <sup>3</sup>He [47, 48] are in agreement within their uncertainties, and are in reasonable agreement with the determination of Ref. [49],

but not with Ref. [50]. We note that if charge symmetry were exact in the three-nucleon systems, the Hamiltonians and polarizabilities of <sup>3</sup>H and <sup>3</sup>He would be identical. Under the charge-symmetry operation that relates the two nuclei the dipole operators in Eqn. (1) would each develop a minus sign, while the radial wave functions and Green's functions would be identical. Most of the chargesymmetry violation in these systems is caused by the repulsive Coulomb interaction between the two protons in <sup>3</sup>He. Note that our uncertainties for these two nuclei are also different. The repulsive Coulomb interaction in <sup>3</sup>He leads to a larger radius for that nucleus, and that may be the source of the larger uncertainty. Matrix elements of infrared operators (i.e., those like the dipole operator that are most sensitive to large distances from the center of a nucleus) converge more slowly in the NCSM than do short-range operators[44, 45].

The uncertainties are even smaller for the calculation in <sup>4</sup>He, which is a very tightly bound system. Our results presented in Table I are significantly smaller than most of the corresponding results, although just at the limit of the estimated uncertainties. We are, however, in good agreement with a recent calculation by Gazit et al.[51], which predicts a slightly smaller polarizability. Note that Ref. [47] used a very primitive nuclear force model and that those results are superseded by those of Ref.[51]. References [52] and [48] used fits to experimental photoabsorption data and Eqn. 2 in order to obtain their results. Values obtained from a direct solution of the Schrödinger equation are therefore at some variance with those calculated using experimental photoabsorption data.

Measurements of  $\alpha$ -particle photoabsorption in the near-threshold region have been controversial over the years, particularly with respect to the height of the cross section at the peak, for which one can find differences of up to a factor of two between different experiments (e.g., see Ref. [36] and references therein). This makes it very challenging to extract an accurate and unambiguous value of the <sup>4</sup>He electric polarizability from the measured <sup>4</sup>He photoabsorption cross section using Eqn. (2). In contrast there has been substantial recent progress in theoretical calculations of the <sup>4</sup>He photoabsorption cross section. Predictions obtained using high precision NN and NNN interaction models (including the ones used in this work) all lie in a rather constrained band [36], in remarkable contrast to the large discrepancies present among different experimental data. This gives us confidence that our prediction for the  $^4\mathrm{He}$  electric polarizability, obtained by direct solution of the Schrödinger equation, will prove to be more accurate than those obtained using existing photoabsorption data.

Since our result of 0.0660(5) fm<sup>3</sup> is obtained with an NNN interaction that overbinds the alpha particle by about 300 keV, it is conceivable that we slightly underestimate  $\alpha_{\rm E}$ . The simplest possible independent-nucleon model for the  $\alpha$ -particle predicts that  $\alpha_{\rm E}$  should scale roughly as the inverse square of the binding energy. Thus,

TABLE I: Values of the electric polarizability of light nuclei, both theoretical and experimental, in units of fm³. The experimental results have been determined by nuclear experiments, including the use of experimental photoabsorption data in Eqn. (2). No uncertainties were given for the ³H, ³He, and ⁴He calculations in [46, 47], but they are likely to be smaller than about 10%. The <sup>6</sup>He result is a hybrid calculation relying on some theoretical input and we add it here for completeness. Results from the present calculation have no listed reference. The result of Ref. [53] for the deuteron is an Effective Field Theory calculation.

Nucleus	$\alpha_{\rm E}^{\rm calc}({\rm fm}^3)$	ref.	$\alpha_{\rm E}^{\rm exp}({\rm fm}^3)$	ref.
$^{2}\mathrm{H}$	0.6328(17)	[20]	0.61(4)	[54]
	0.6314(19)	[53]	0.70(5)	[55]
$^{3}\mathrm{H}$	0.139(2)		_	
	0.139	[46]		
$^{3}{\rm He}$	0.149(5)		0.250(40)	[50]
	0.145	[47]	0.130(13)	[49]
	0.153(15)	[48]		
<sup>4</sup> He	0.0660(5)		0.072(4)	[52]
	0.0673(5)		0.076(8)	[48]
	0.0655(4)	[51]		
	0.076	[47]		
<sup>6</sup> He			1.99(40)	[48]

even our calculations that neglect three-nucleon forces in the alpha particle result in a value of  $\alpha_{\rm E}=0.0822(5)~{\rm fm^3}$  (25% higher than our best result that incorporates these forces), while reducing the binding energy from 28.6 to 25.4 MeV (an 11% decrease). A similar effect is also seen in the <sup>3</sup>He and <sup>3</sup>H calculations, where our three-nucleon forces had been adjusted so that calculated binding energies differ from experiment by no more than one part per thousand. We have even considered another model, in which the three-body system is described with the same accuracy, but in which the alpha particle is overbound by only about 200 KeV, and in this case we obtain 0.0673(5) fm<sup>3</sup>. This would not explain the large differences (al-

though with large uncertainties) in Table I between direct calculations of  $\alpha_{\rm E}$  from the Schrödinger equation and those using photoabsorption data and Eqn. (2). We estimate that improving further the description of the binding energy of <sup>4</sup>He would not affect the electric polarizability by more than 2%, so that we recomend the value of 0.0677(8) fm<sup>3</sup>.

#### IV. CONCLUSION

We have used the latest generation NN and NNN interactions in a NCSM framework in order to obtain accurate three- and four-nucleon solutions of the Schrödinger equation. Using the Lanczos-moment method to implement Podolsky's technique [40] for treating second-order perturbation theory, we have calculated the electric polarizabilities of <sup>3</sup>H, <sup>3</sup>He, and <sup>4</sup>He. Our result for <sup>3</sup>H is in excellent agreement with that of Ref. [46], while that for <sup>3</sup>He is in good agreement with previous work. Our recommended value of 0.0677(8) fm<sup>3</sup> for <sup>4</sup>He is at the lowest end of the calculations that used experimental photoabsorption data directly in Eqn. (2), and is in reasonable agreement with a more recent calculation using modern phenomenological potentials. Future calculations for other light nuclei such as <sup>6</sup>He and <sup>6</sup>Li should be tractable, but would require a change of basis for the NCSM. For nuclei with mass numbers greater than five, a Slater Determinant basis is much more efficient than the relative coordinate approach used in this work.

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